# Topological Physics in Band Insulators


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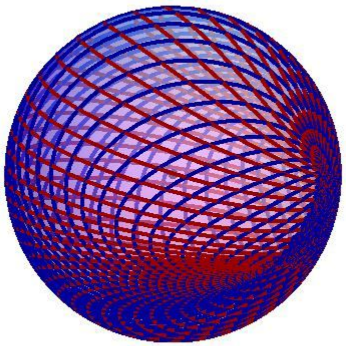

# Lecture Topics:

1. Topological Band Insulators (mostly 1D)
2. Topological Insulators (2D and 3D)
3. Low energy models for real materials
4. Wannier representations and band projectors

# Collaborators:

**Charlie Kane**
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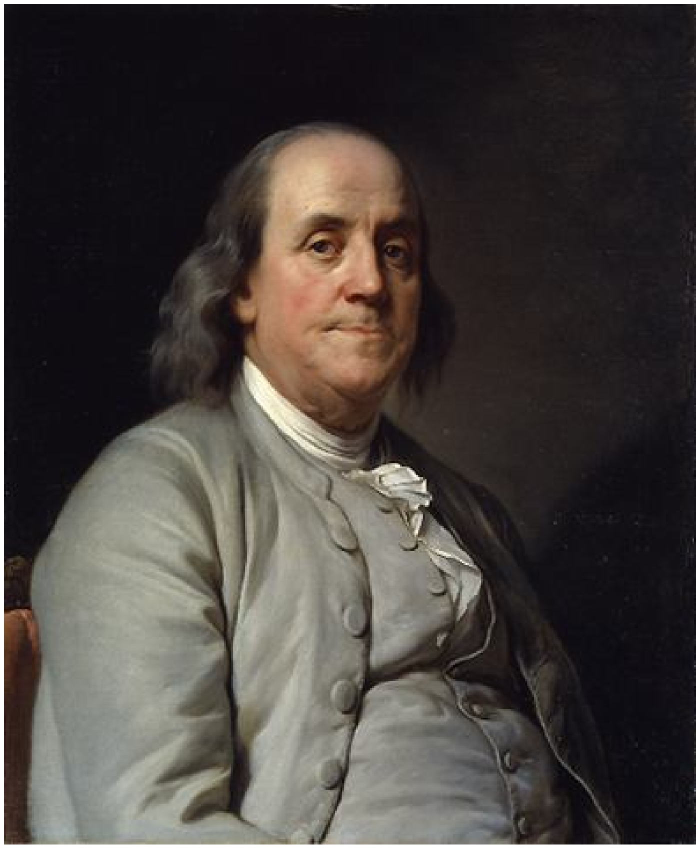
**Petr Kral**
**Andrew Rappe**
**Michael Rice**
**Saad Zaheer**
**Fan Zhang**

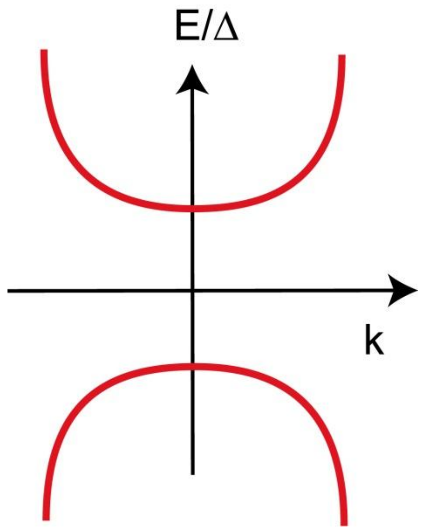
# Electronic States of Matter

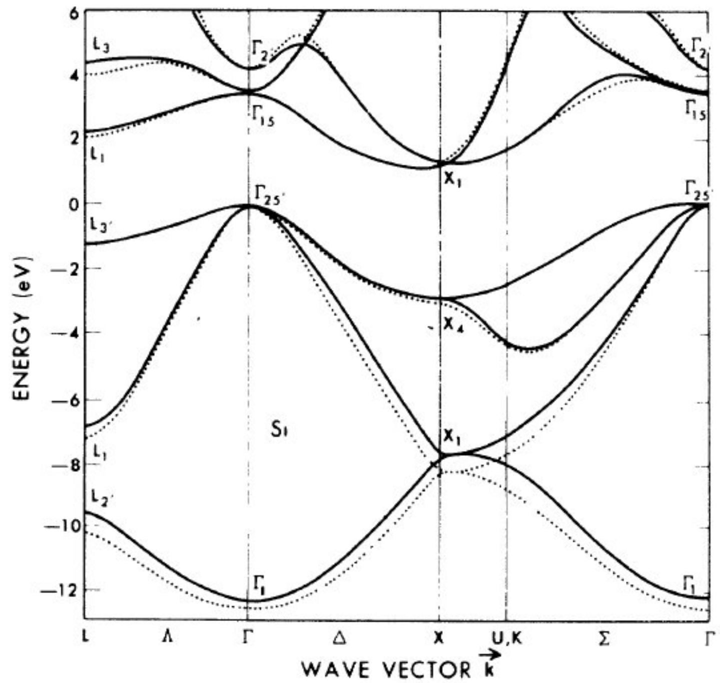
## Benjamin Franklin (University of Pennsylvania)



***That the Electrical Fire freely removes from Place to Place in and thro' the Substance of a Non-Electric, but not so thro' the Substance of Glass. If you offer a Quantity to one End of a long rod of Metal, it receives it, and when it enters, every Particle that was before in the Rod pushes it's Neighbour and so on quite to the farther End where the Overplus is discharg'd… But Glass from the Smalness of it's Pores, or stronger Attraction of what it contains, refuses to admit so free a Motion. A Glass Rod will not conduct a Shock, nor will the thinnest Glass suffer any Particle entring one of it's Surfaces to pass thro' to the other.***

# Band Insulators (orthodoxy)

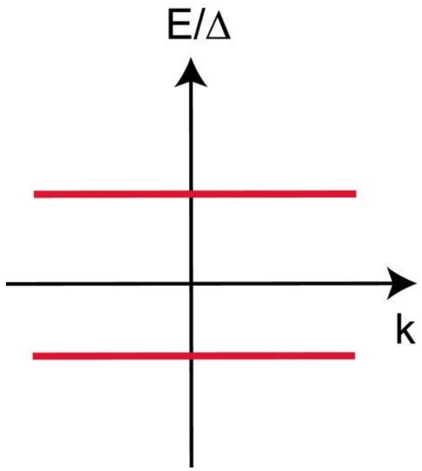


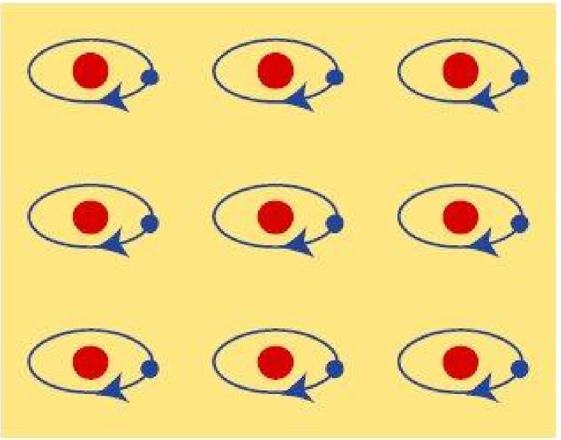




Examples: Si, GaAs, $SiO_{2,}$ etc

Because of the “smallness of its pores”

# Band Insulators (atomic limit)



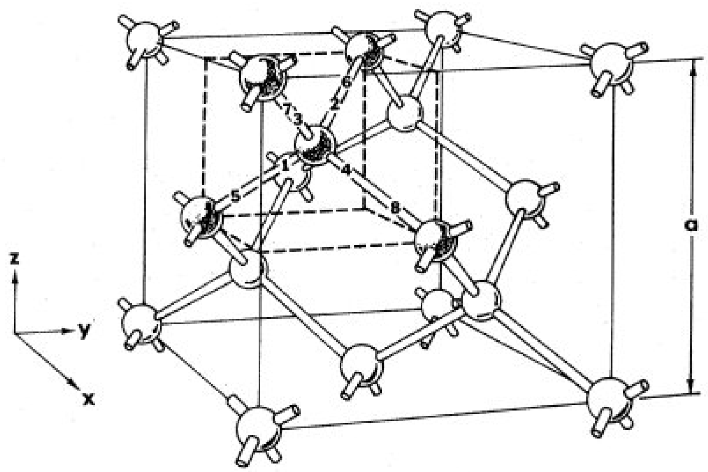



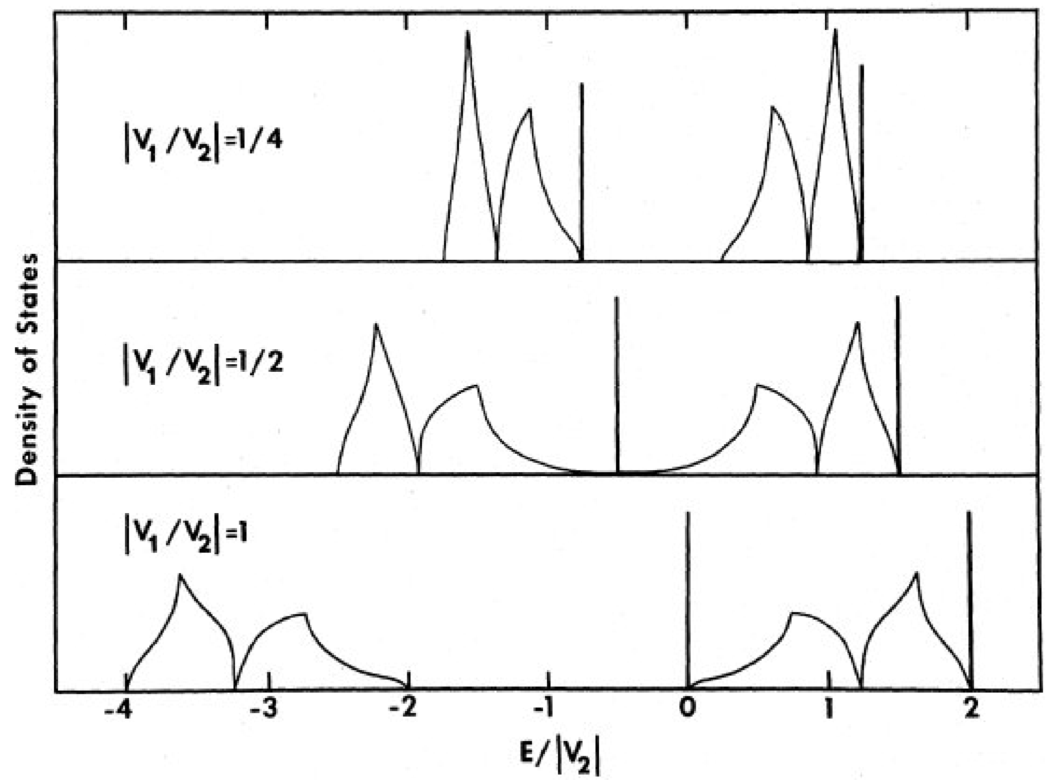
Examples: atoms, molecular crystals, etc.

"Attraction for what it contains"

# Transition from covalent to atomic limits

Tetrahedral semiconductors

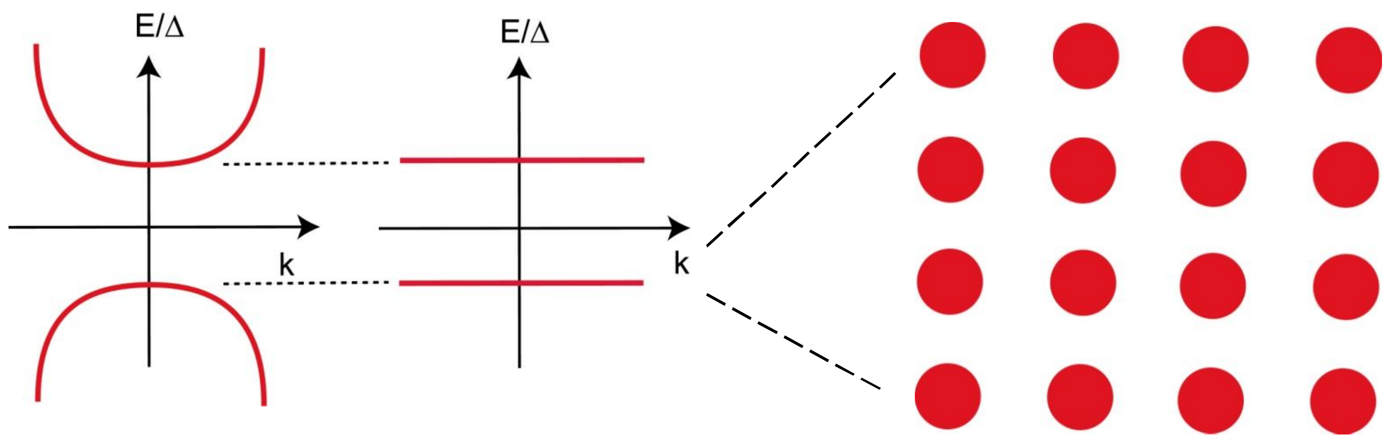



Weaire & Thorpe (1971)

# Modern view: Gapped electronic states are equivalent

**Kohn (1964):** insulator is exponentially insensitivity to boundary conditions



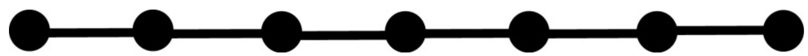

weak coupling    strong coupling    “nearsighted”, local

Postmodern: Gapped electronic states
are distinguished by topological invariants

# Topological States

Topological classification of valence manifold

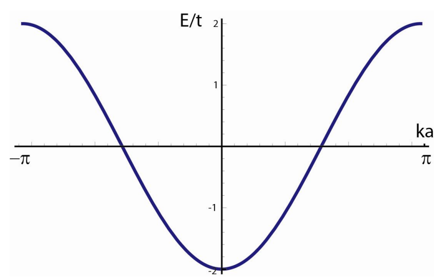
Examples in 1D lattices: variants on primer



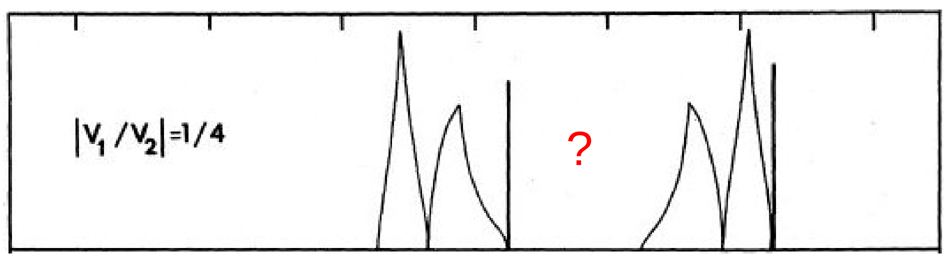
saturated

$$H = t\sum_n c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1}$$

$$= \sum_k 2t\cos ka$$




empty



# Cell Doubling (Peierls, SSH)

$$H(k) = \begin{pmatrix} 0 & t_1 + t_2 e^{-2ika} \\ t_1 + t_2 e^{2ika} & 0 \end{pmatrix}$$

smooth gauge $$H(k + \frac{2\pi}{2a}) = H(k)$$

$$H(k) = \vec{h}(k) \cdot \vec{\sigma} \qquad \begin{cases} h_x = t_1 + t_2 \cos 2ka \\ h_y = t_2 \sin 2ka \\ h_z = 0 \end{cases}$$

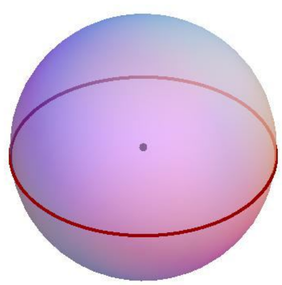
Su, Schrieffer, Heeger (1979)

# Project onto Bloch Sphere

$$H = |h(k)|\vec{d}(k) \cdot \vec{\sigma}$$

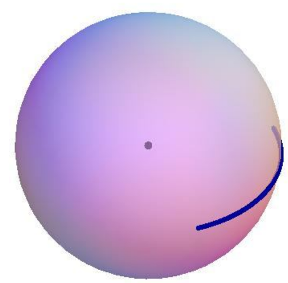
$$|h(k)| = \sqrt{t_1^2 + t_2^2 + 2t_1 t_2 \cos 2ka}$$

$$t_2 > t_1$$



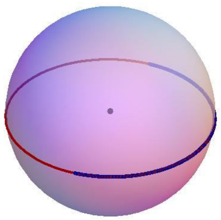
Closed loop

$$t_1 > t_2$$



Retraced path

# Formulation as a Berry's Phase



$$\psi_- = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -e^{i\phi} \end{pmatrix}; \psi_+ = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{i\phi} \end{pmatrix}$$

$$\mathrm{Im}\left\langle \psi_\lambda \,\middle|\, \frac{\partial \psi_\lambda}{\partial \lambda} \right\rangle = \frac{\partial \gamma}{\partial \lambda} \qquad \psi_\lambda = e^{i\gamma}\left|\psi_\lambda\right|$$

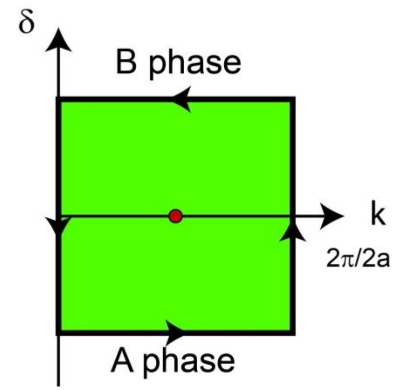
$$\gamma = \oint \frac{\partial \gamma}{\partial \phi}\, d\phi \qquad \begin{cases} \pi: \ \text{A phase} & \text{Closed loop} \\ 0: \ \text{B phase} & \text{Retraced path} \end{cases}$$

# Formulation using Electric Polarization

$$\vec{h}(k) \Rightarrow \vec{h}(k,\delta)$$

$$\delta = t_1 - t_2$$

$$\vec{\lambda} = (k,\delta)$$



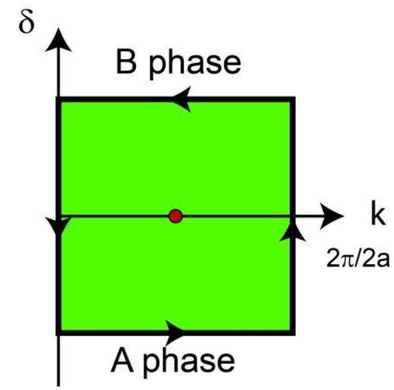

$$\gamma_A - \gamma_B = \mathrm{Im} \oint \underbrace{\left\langle \psi \,\middle|\, \frac{\partial \psi}{\partial k} \right\rangle}_{A_k\,:\ \text{connection}} dk$$

# Stokes Integral of Berry Curvature

$$\vec{h}(k) \Rightarrow \vec{h}(k,\delta)$$

$$\delta = t_1 - t_2$$

$$\vec{\lambda} = (k,\delta)$$




$$\gamma_A - \gamma_B = \int_S \underbrace{\mathrm{Im}\left\{\left\langle \frac{\partial\psi}{\partial\delta} \,\middle|\, \frac{\partial\psi}{\partial k}\right\rangle - \left\langle \frac{\partial\psi}{\partial k} \,\middle|\, \frac{\partial\psi}{\partial\delta}\right\rangle\right\}}_{F_{k,\delta}} d^2\lambda$$

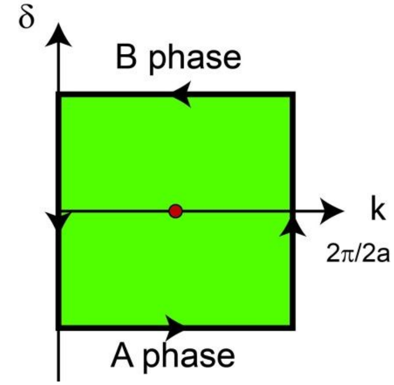
$F_{k,\delta}$ Berry curvature

# Polarization from adiabatic current

$$\vec{h}(k) \Rightarrow \vec{h}(k,\delta)$$

$$\delta = t_1 - t_2$$

$$\vec{\lambda} = (k,\delta)$$




$$\gamma_A - \gamma_B = \begin{cases} \dfrac{\Omega}{2} \\ \dfrac{2\pi}{e}\displaystyle\int dt\,\langle J \rangle_\delta = \dfrac{2\pi}{eL}(P_A - P_B) \end{cases}$$

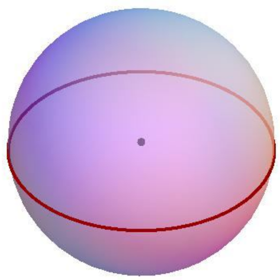
$\Omega:$ Solid angle swept out

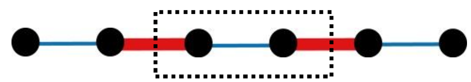
$\langle J \rangle_\delta$ Ground state current (via Kubo)

King-Smith and Vanderbilt (1993)

# Example: dimerized 1D lattice

$t_2 > t_1$

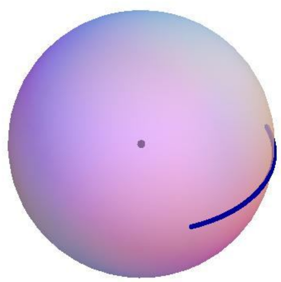


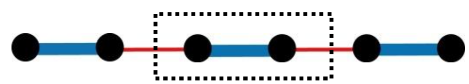


$$\gamma = \pi$$

$$P = \pm \frac{e}{2}$$ (spinless)

$t_1 > t_2$





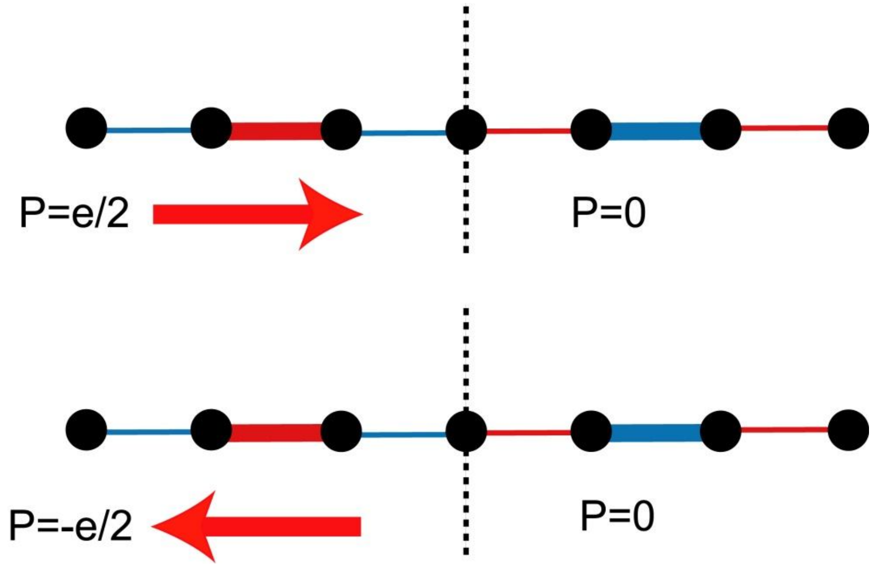
$$\gamma = 0$$

$$P = 0 \quad (ne)$$

$$\left. \begin{array}{l} \Omega \to \Omega + 4\pi \\ \gamma \to \gamma + 2\pi \\ P \to P + e \end{array} \right\}$$

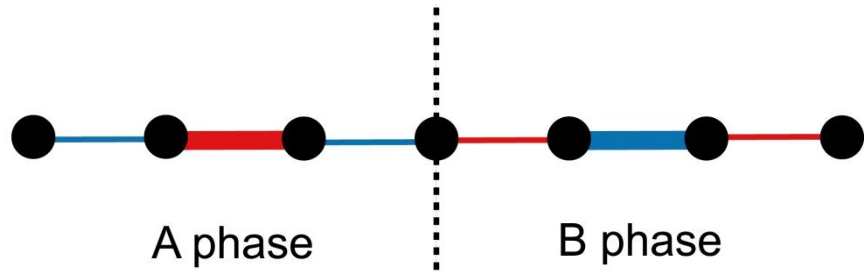
displaces a single charge across each unit cell

# Topological Domain Walls




$$Q^{*} = \pm \frac{e}{2}$$ (spinless)

# State Counting

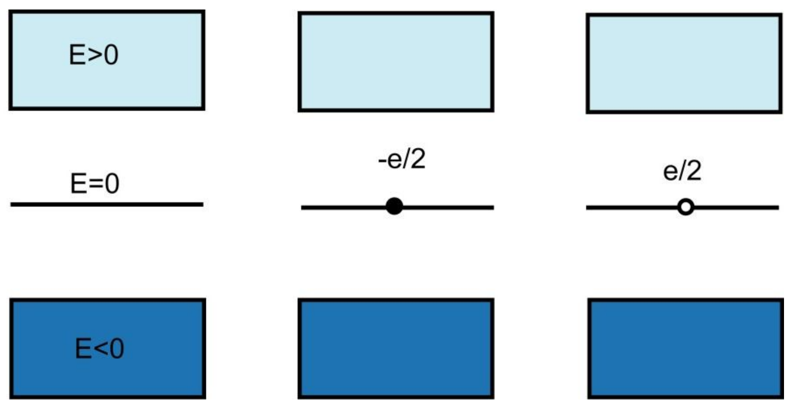



Particle-hole symmetry

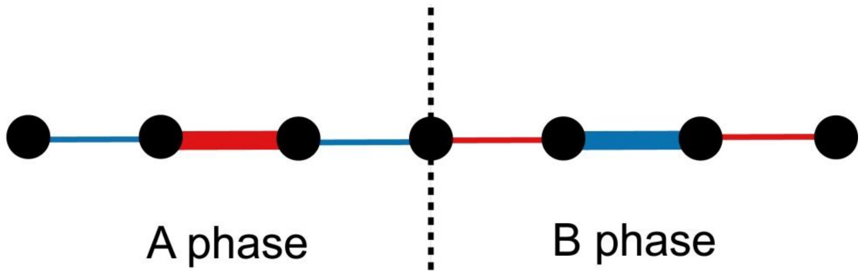
$$C\;H\;C^{-1} = -H; \quad C = \sum_n (-1)^n c_n^\dagger c_n$$

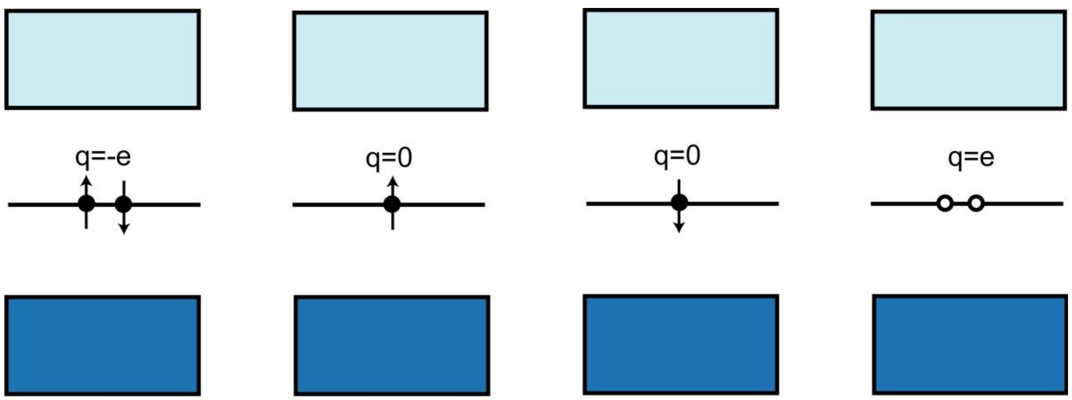
on odd numbered chain

self conjugate state
on one sublattice



# ...with spin



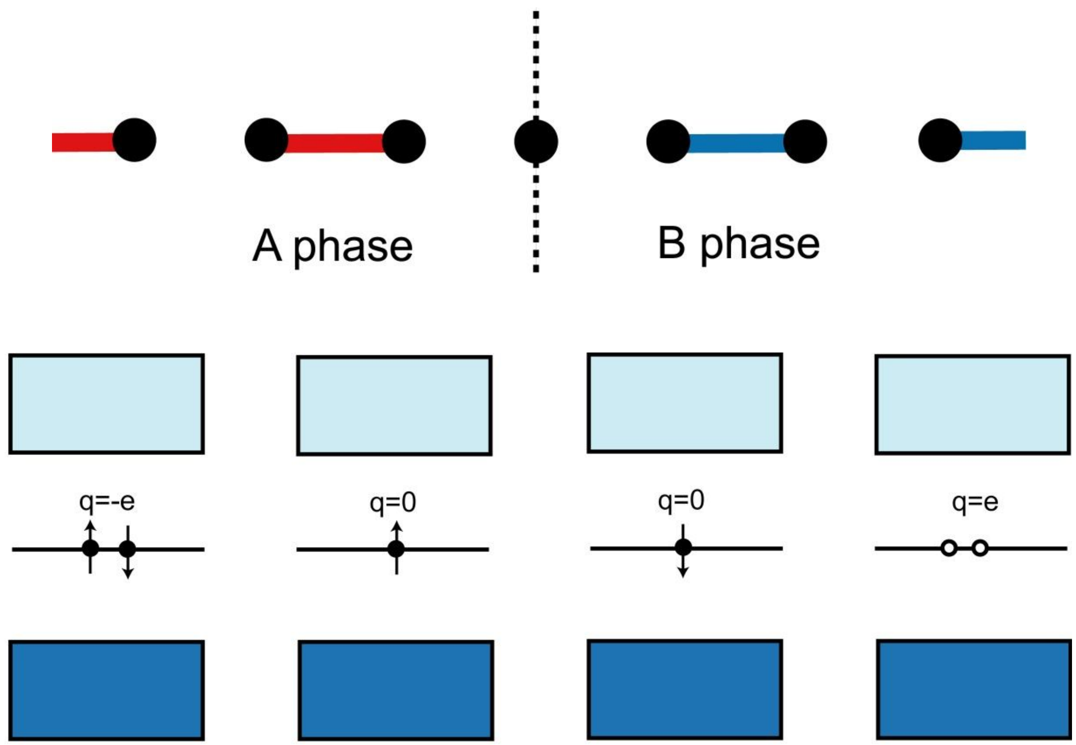




spin-less charge

charge-less spins

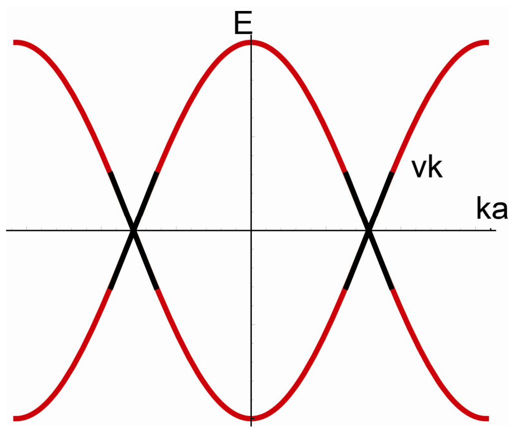
spin-less charge

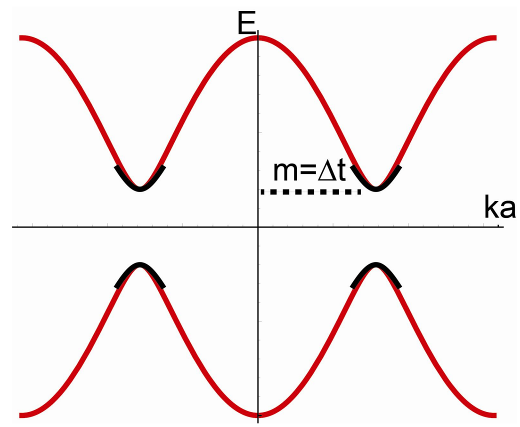
# ...for strong coupling




spin-less charge charge-less spins spin-less charge

# Continuum Model



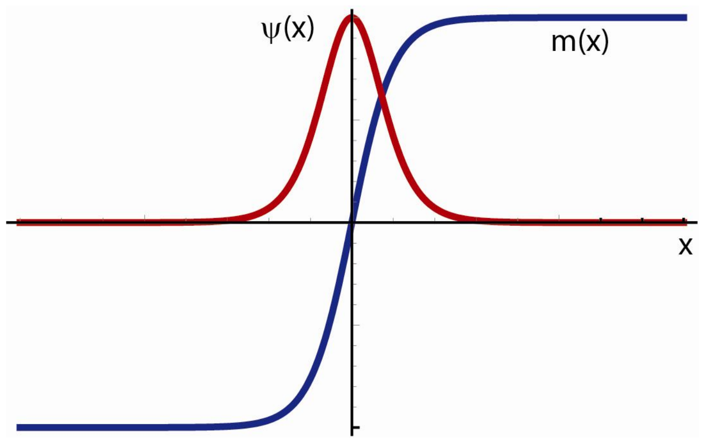




$$\begin{pmatrix} e^{-\frac{i\pi}{4}} & 0 \\ 0 & e^{\frac{i\pi}{4}} \end{pmatrix} H\left(\frac{\pi}{2a}+q\right)\begin{pmatrix} e^{\frac{i\pi}{4}} & 0 \\ 0 & e^{-\frac{i\pi}{4}} \end{pmatrix} = -iv_F\hat{\sigma}_x\frac{\partial}{\partial x}+m\hat{\sigma}_y$$

$$E = \pm\sqrt{m^2+v^2q^2}$$

"relativistic bands" back-scattered by mass $m = t_1 - t_2$

# Mass inversion at  domain wall



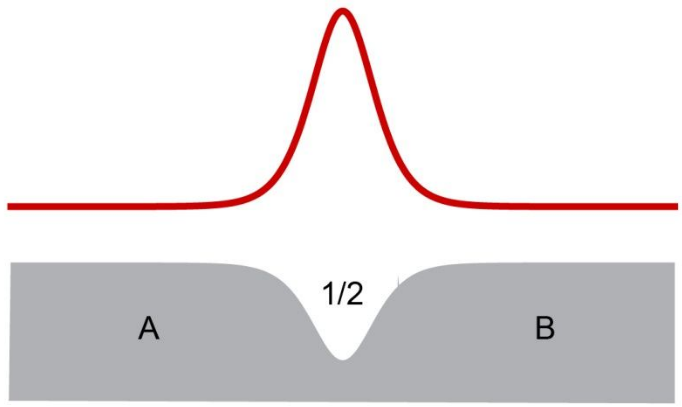

Sublattice-polarized E=0 bound state

$$\psi(x) = A\exp\left[-\int_0^x \frac{m(x)}{v}\,dx\right]\begin{pmatrix}0\\1\end{pmatrix} \qquad \xi = \frac{\hbar v}{m}$$

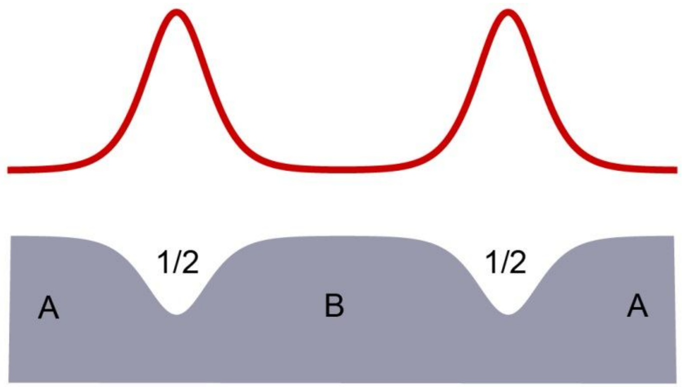
Jackiw-Rebbi (1976)

# Backflow of filled Fermi sea

Fractional depletion
of filled Fermi sea




Occurs in pairs
(topologically connected)



# Heteropolar Lattice

$$H = t\sum_n c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1}$$

$$+\,\delta\sum_n (-1)^n (c_{n+1}^\dagger c_n + c_n^\dagger c_{n+1}) + \Delta\sum_n (-1)^n c_n^\dagger c_n$$

modulate bond strength

staggered potential

Rice and GM (1982)

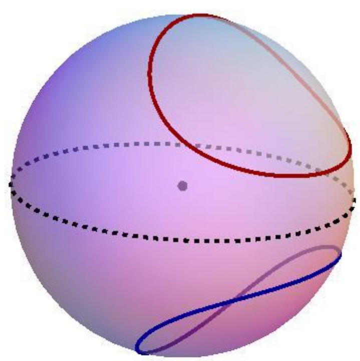
# On Bloch Sphere

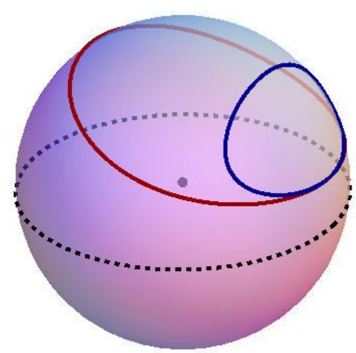
$$H(k) = \vec{h}(k) \cdot \vec{\sigma} \quad \begin{cases} h_x = t + \delta + (t - \delta)\cos 2ka \\ h_y = (t - \delta)\sin 2ka \\ h_z = \Delta \end{cases}$$

$\Delta > 0$

$\Delta < 0$

$\delta > 0$



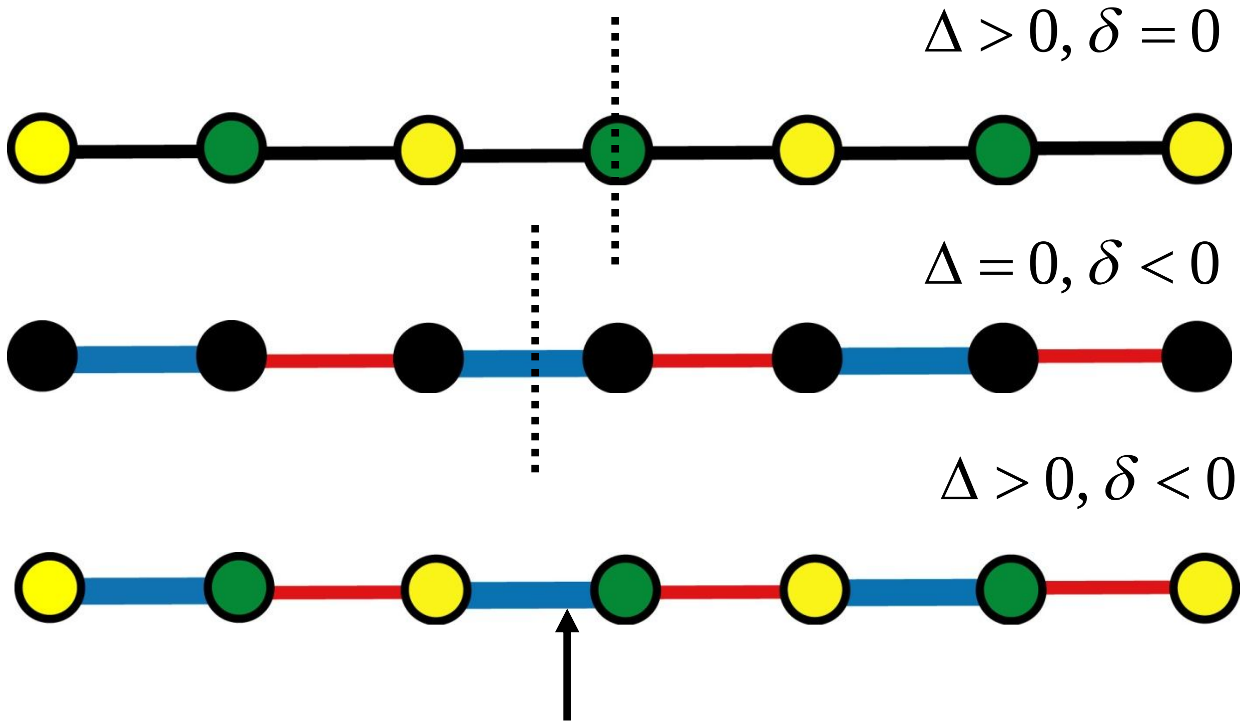


$\delta > 0$

$\delta < 0$

$\Delta > 0$

# High symmetry cases

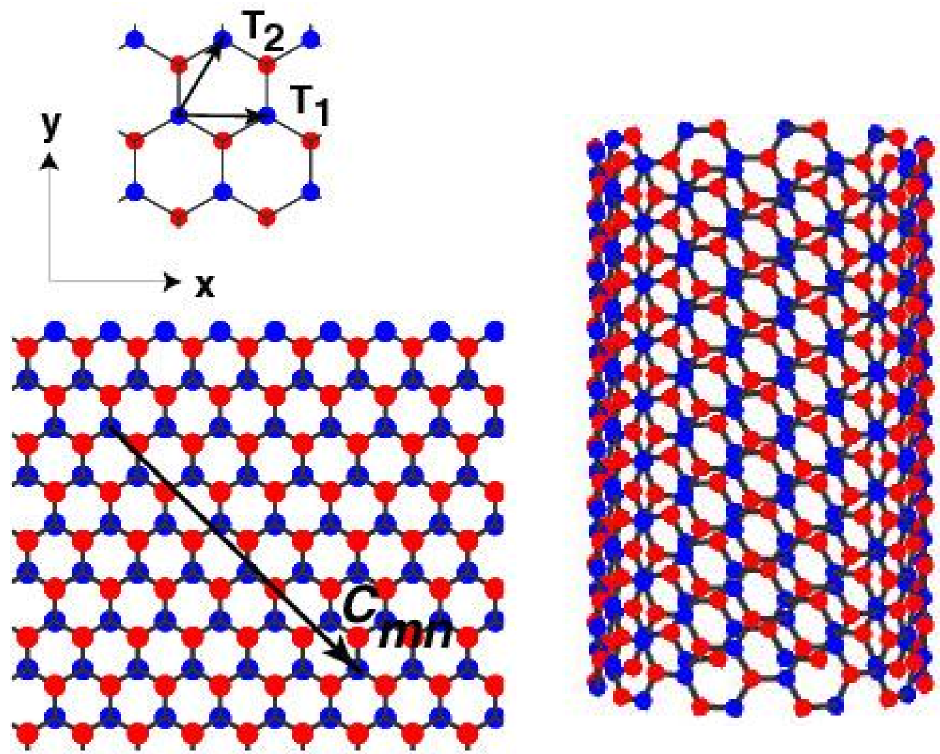



Continuously tunes the domain wall  charge

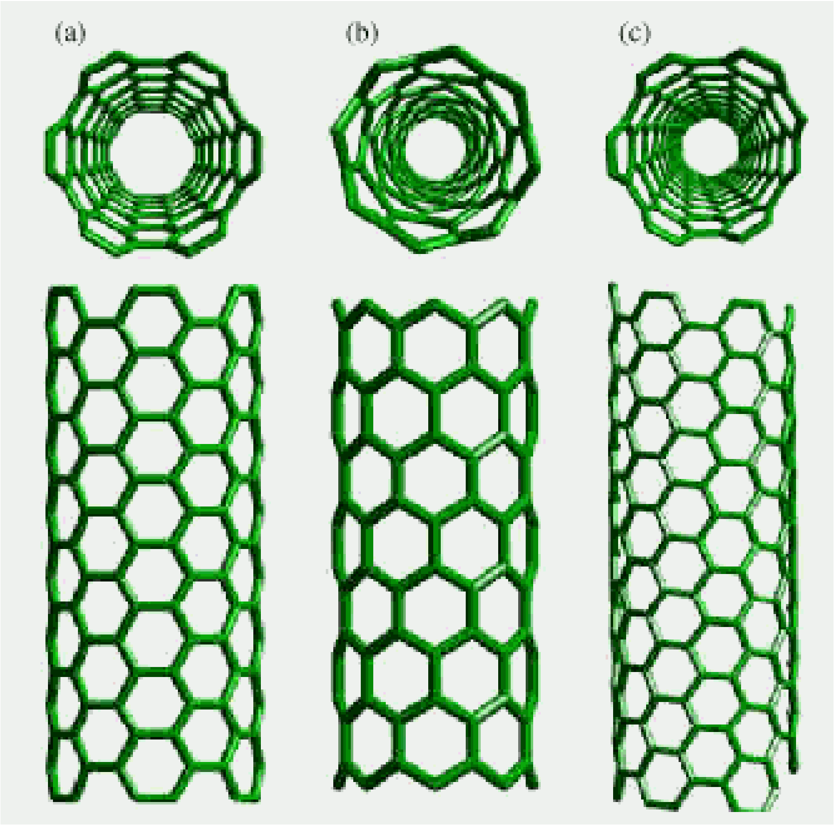
$$Q^{*} = ne + Q_{v}(\delta, \Delta)$$

# Heteropolar NT's of Boron Nitride

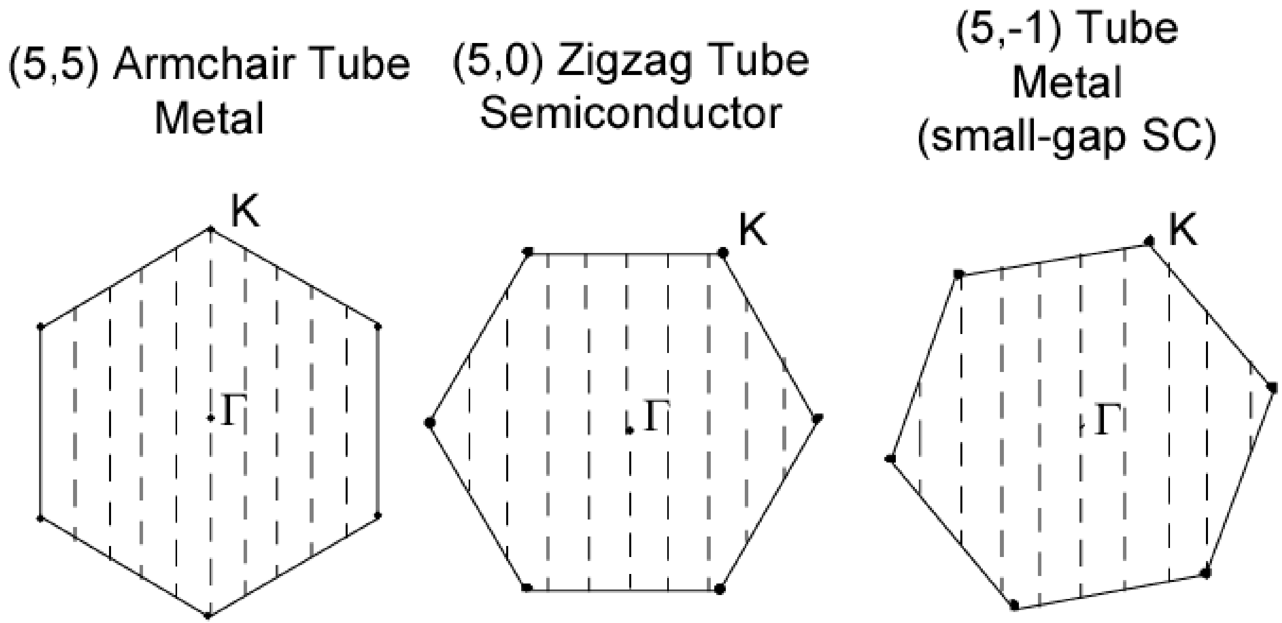
BN is the III-V variant of graphene. The B and N occupy different sublattices -- this lowers the symmetry and leads to new physical effects



# Conducting v. Semiconducting Nanotubes



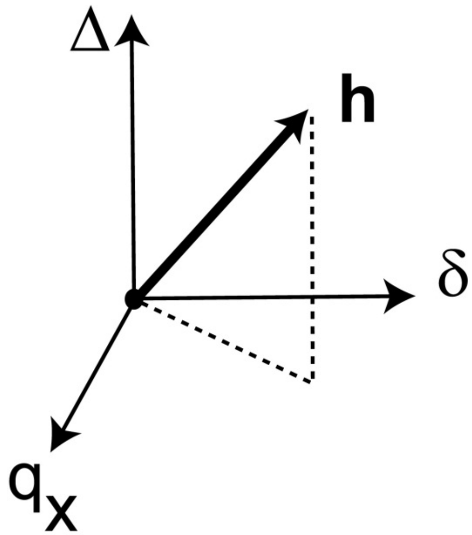
# Conducting v. Semiconducting Nanotubes



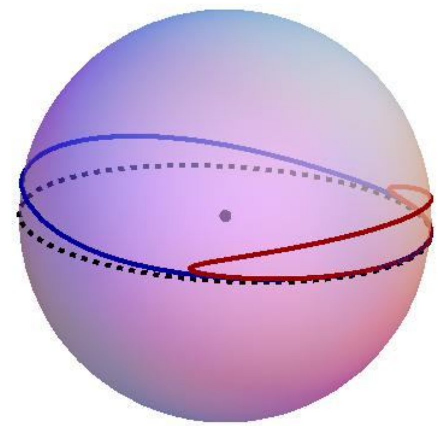

**m=n** **mod(m-n,3) = ±1** **mod(m-n,3) = 0, m≠n**

# Nanotube Polarization

ionicity



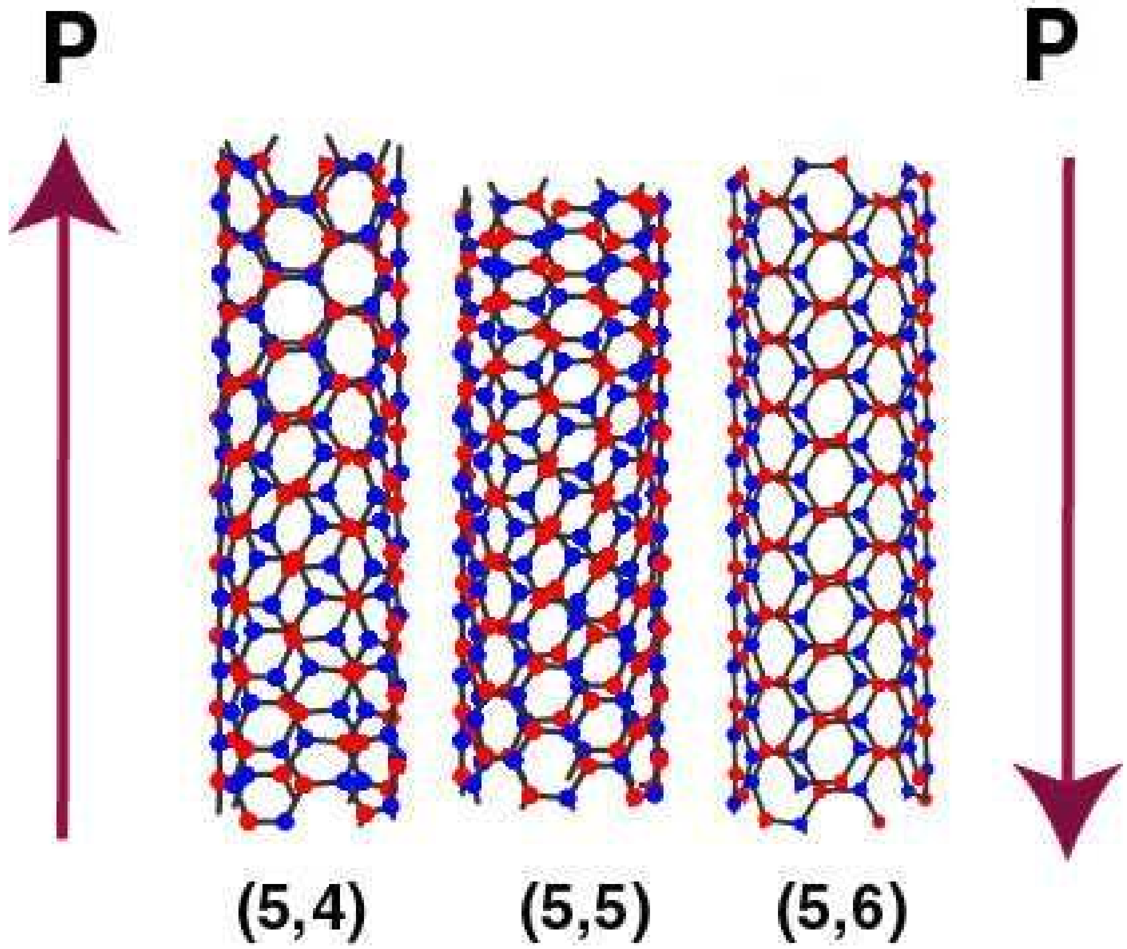

chirality



$$P = e\frac{\gamma}{2\pi}, \qquad \frac{\pm e}{2} - e\frac{\gamma}{2\pi}$$

$$H(q_x,\delta,\Delta) = \Psi^{\dagger}\begin{pmatrix} \Delta & \hbar v_F(q_x - i\delta) \\ \hbar v_F(q_x + i\delta) & -\Delta \end{pmatrix}\Psi$$

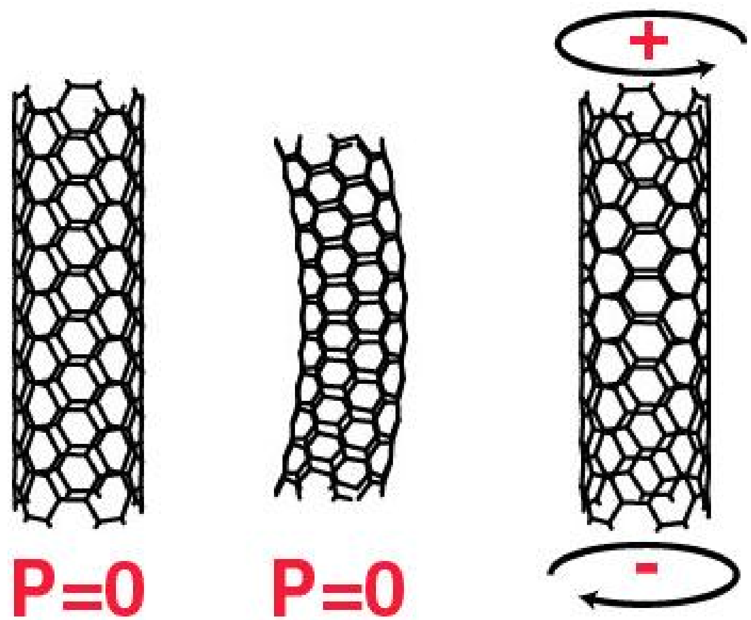
# Nanotube Polarization




GM and P. Kral (2002)

# Polarization and elastic strain

(twist is a gauge field that modulates $\delta$)

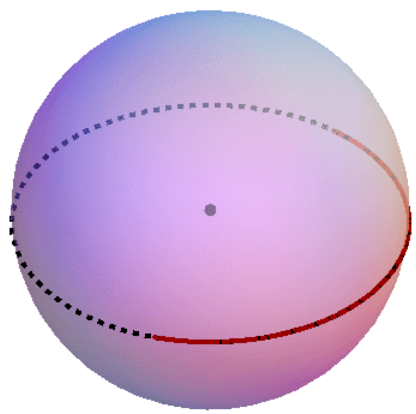



Heteropolar NT's are molecular piezoelectrics

GM and P. Kral (2002)

# **One Parameter Cycle**

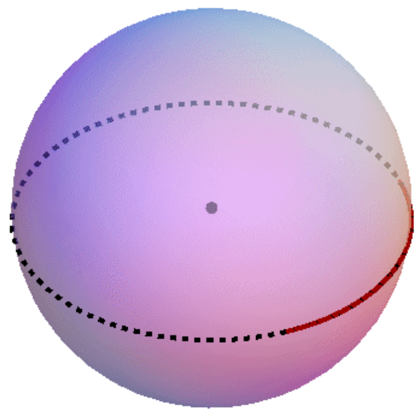
e.g. periodic tube torsion modulates P



Bond strengths are modulated periodically
in a reversible cycle

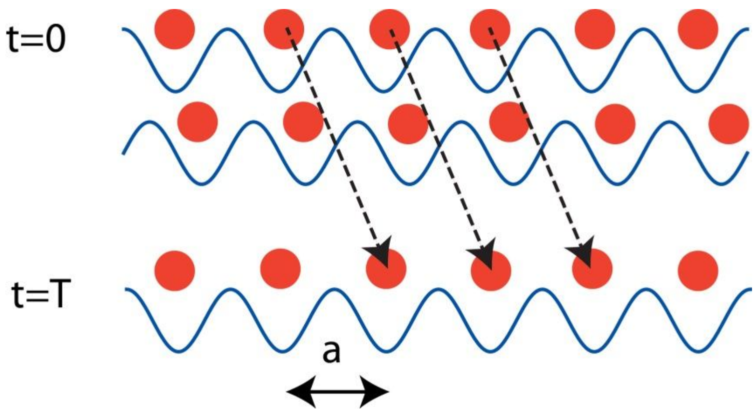
# Two Parameter Cycle

ionicity and chirality are
nonreciprocal potentials



Nonreciprocal cycle enclosing a point of degeneracy with Chern number: $$n = \frac{1}{4\pi}\int_S dk\, dt \left[ \vec{d}(k,t) \cdot \left( \partial_k \vec{d} \times \partial_t \vec{d} \right) \right]$$

# Thouless Charge Pump




$$H(k,t+T)=H(k,t)$$

with no gap closure on path

$$\Delta P=\frac{e}{2\pi}\left(\int_{t+T} A_k\ dk-\int_{t} A_k\ dk\right)$$

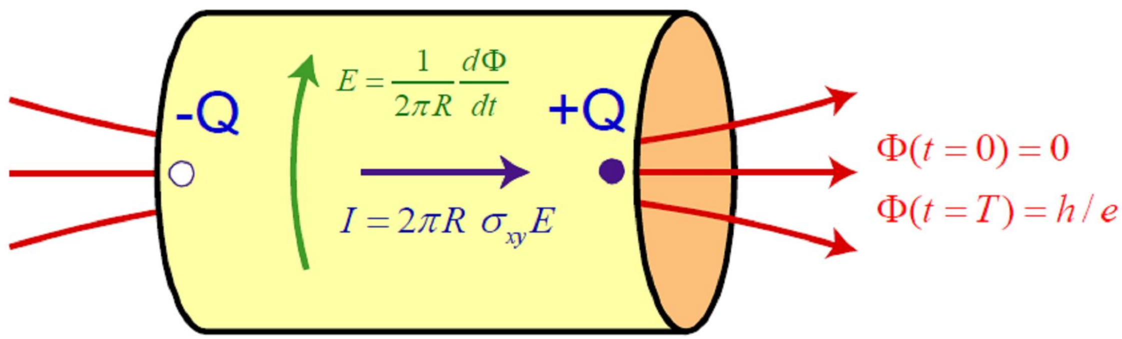
$$=\frac{e}{2\pi}\int_S F_{k,t}\ dk\ dt=ne$$

n=0 if potentials commute

Thouless (1983)

# Quantized Hall Conductance

Adiabatic flux insertion through 2DEG on a cylinder:




$$2\pi R \int dt \left\langle j \right\rangle = 2\pi R \int dt\ \sigma_{xy} E = Q$$

$$\sigma_{xy} \frac{h}{e} = Q = ne$$

$$\sigma_{xy} = n \frac{e^2}{h}$$

TKNN invariant
is the Chern number

Laughlin (1981), Thouless et al. (1983)

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